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Contents

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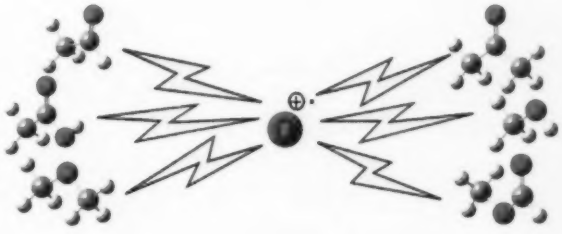
Gas-phase organic reactions of the atomic oxygen radical cation

Charles M. Nichols, Zhibo Yang, Veronica M. Bierbaum

● The atomic oxygen radical cation is abundant in many environments. ● Reactivity of $O^{\bullet+}$ with several organic compounds has been studied with a FA-SIFT. ● Efficient charge transfer, often with fragmentation, is a dominant mechanism. ● Additional reactions include attack on carbonyl and methyl groups. ● RRKM and electronic structure calculations provide insight into the reactions.

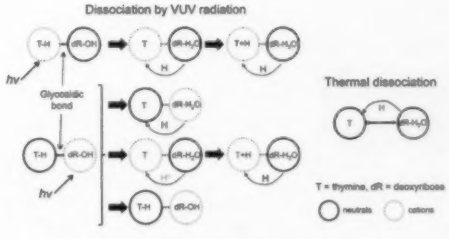


7–11

Fragmentation of thymidine induced by ultraviolet photoionization and thermal degradation

H. Levola, K. Kooser, E. Rachlew, E. Nõmmiste, E. Kukk

● The main fragments after photoionization are deoxyribose- and thymine-based. ● Thermal decomposition of thymidine is observed to start around 138°C. ● Degradation process is explained by the rupture of glycosidic bond. ● Appearance energies of thymidine and its fragments did not depend on temperature.

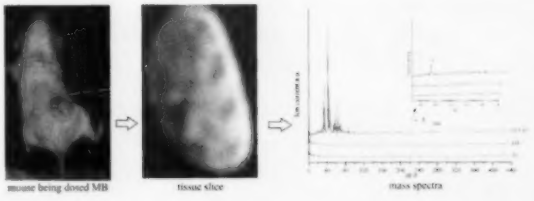


12–18

In situ detection of methylene blue in tissues by laser desorption vacuum ultraviolet single photon postionization mass spectrometry

Qing Yang, Yongjun Hu, Yanchun Wei, Honglei Wang, Jiwen Guan, Yanjiao Zhang, Shaoxin Li

● Medicinal chemicals (taking the methylene blue (MB) as the example) in situ in intact tissues has been observed by laser desorption postionization mass spectrometry with 10.5 eV vacuum ultraviolet single photon ionization. ● The experiment shows the optimal delay time between the desorption laser and ionization laser was 18–35 μs. ● The detections of amino acids fragments and other biological species in the tissue do not interfere with the signal of MB detected in the MB-dosed tissue.



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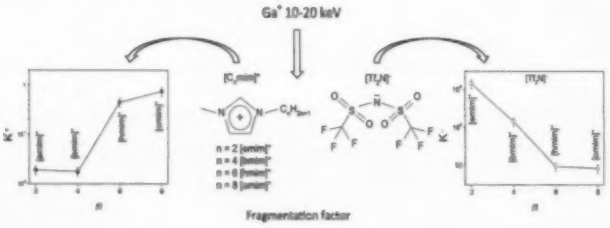
19–25

Ion-induced fragmentation of imidazolium ionic liquids: TOF-SIMS study

Nenad Bundaleski, Stefano Caporali, Sergey P. Chenakin, Augusto M.C. Moutinho, Orlando M.N.D. Teodoro, Alexander Tolstogouzov

● Positive and negative TOF-SIMS spectra by 10–20 keV Ga^+ bombardment of $[C_nmim][Tf_2N]$, where n = 2, 4, 6, 8, were measured. ● The predominant peaks were intact cation $[C_nmim]^+$ and anion fragment F^-. ● The sum intensity of positive cation fragments increased with an increase in the alkyl chain length (n-value). ● Ion-induced fragmentation of anion decreased with an increase of the n-value and with a decrease in the projectile energy.

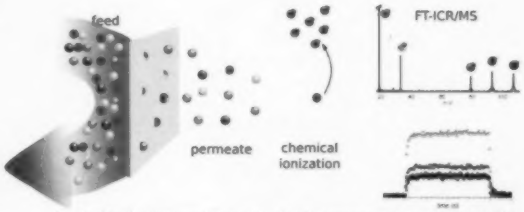


26–35

Characterization of a membrane inlet interfaced with a compact chemical ionization FT-ICR for real-time and quantitative VOC analysis in water

Essyllt Louarn, Anissa Hamrouni, Christophe Colbeau-Justin, Léa Bruschi, Joël Lemaire, Michel Heninger, Hélène Mestdagh

● A compact FT-ICR/MS was successfully interfaced to an MIMS system for water analysis. ● The dependence of the pervaporation on temperature and pressure was investigated. ● The enrichment factors for 5 VOCs were calculated and ranged from ten to several thousand. The observed signal response times (t_{10-90}) were less than 1 min. ● The results were dependent on the solubility and the mass of the compounds. ● The setup enabled quantitative analysis in real-time.



36–41

Modeling of an ion source lens system for sensitivity enhancement in a non-scanning linear ion trap

Boris Brkić, Stamatios Giannoukos, Neil France, Aurika Janulyte, Yves Zerega, Stephen Taylor

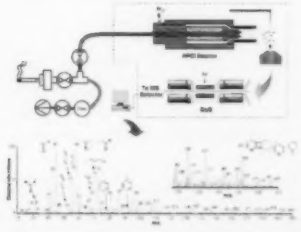
● We present experimental selective mass isolation for a linear ion trap (LIT) operating in a non-scanning mode. ● Ion source lens system (ISLS) coupled to a non-scanning LIT was simulated using CPO program. ● Simulation study of ion injection, trapping and ejection was done to optimize LIT sensitivity. ● Our results have shown that an optimized ISLS can improve LIT sensitivity by a factor of 4 compared to commercial ion source lens systems.

42–48

Application of direct atmospheric pressure chemical ionization tandem mass spectrometry for on-line analysis of gas phase of cigarette mainstream smoke

Cheng-Yong Jiang, Shi-Hao Sun, Qi-Dong Zhang, Yu-Ping Ma, Hui Wang, Jian-Xun Zhang, Yong-Li Zong, Jian-Ping Xie

● A novel direct APCI–MS/MS method has been developed for on-line analysis of MSS. ● Smoking procedure was carried out using a modified commercial smoking machine. ● The APCI source was modified to allow the direct introduction of MSS samples. ● The developed method could achieve on-line analysis of puff-by-puff MSS. ● Advantages of the method: simplicity, high speed, good sensitivity and repeatability.

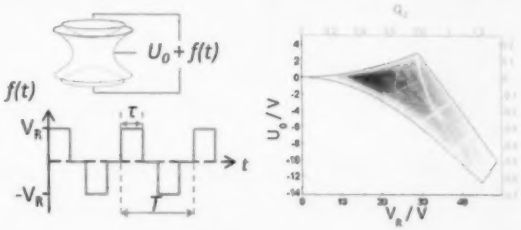


49–53

The 3-state digital ion trap

Steffi Bandelow, Gerrit Marx, Lutz Schweikhard

● A Paul trap operated with a 3-state digital driving signal is introduced. ● A mathematical description based on Fourier analysis is presented. ● Stability diagrams are measured for different duty cycles. ● This operating scheme can be used for interaction studies.

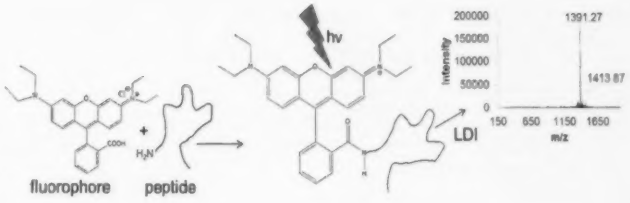


54–59

Fluorophore-assisted laser desorption/ ionization-mass spectrometry (FALDI-MS)

Raymond E. West III, Eric W. Findsen, Dragan Isailovic

● Direct analysis of fluorescently labeled peptides by LDI-MS is demonstrated for the first time. ● Peptides labeled on their N-termini with rhodamine B were analyzed by FALDI MS and MS/MS without the addition of a matrix. ● MS/MS spectra of fluorescently labeled peptides show exclusively a and b ion series enabling easier peptide sequencing. ● FALDI-MS allows for selective ionization of the fluorescently labeled peptides in peptide mixtures.

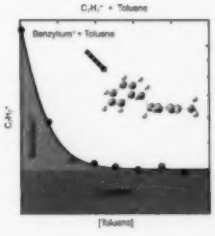


60–66

Temperature dependences for the reactions of Ar^+, O_2^+, and $C_7H_7^+$ with toluene and ethylbenzene

Joshua J. Melko, Shaun G. Ard, Nicholas S. Shuman, Albert A. Viggiano

● Ar^+ and O_2^+ react with alkylbenzenes near the collision rate, with little T-dependence. ● $C_7H_7^+$ is the primary product, which we find exists mainly as the benzylium isomer. ● The benzylium isomer reacts through clustering, R-group transfer, and thermal activation. ● The benzylium-cluster product has a calculated bond energy of about 15 kcal mol^{-1}.



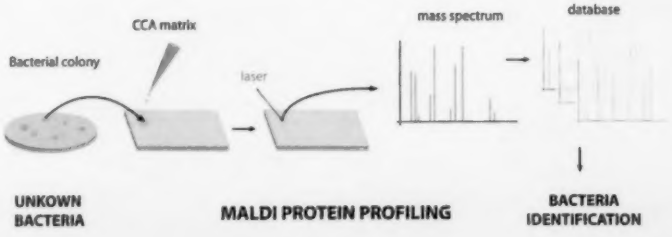
Review Article

67–79

Identification of bacteria using mass spectrometry techniques

Lukáš Krásný, Radovan Hynek, Igor Hochel

● We summarize development and innovations in MS identification of bacteria. ● We compare current commercial systems designed for clinical use. ● We review biomarkers suitable for identification of bacteria by MS.



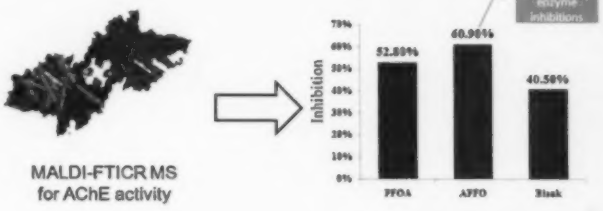
Short Communications

80–83

Effect of ammonium perfluorooctanoate on acetylcholinesterase activity and inhibition using MALDI-FTICRMS

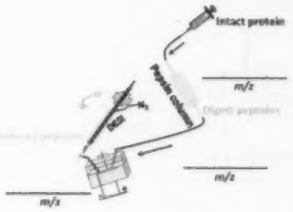
Tingting Cai, Li Zhang, Rong Wang, Chen Liang, Yurong Zhang, Yinlong Guo

● The effect of APFO and PFOA on AChE activity and inhibition had been investigated. ● MALDI-FTICRMS was used to detect the activity of AChE. ● AChE inhibitions from irreversible inhibitor were increased by adding APFO and PFOA. ● APFO and PFOA had no obvious effect on AChE inhibitions from reversible inhibitor.



84–92

Integration of online digestion and electrolytic reduction with mass spectrometry for rapid disulfide-containing protein structural analysis

Qiuling Zheng, Hao Zhang, Hao Chen

● Online digestion, electroreduction and DESI-MS are combined for protein structural analysis. ● It takes <7 min to detect digested and reduced peptides. ● Selective reduction can be achieved using different reduction potentials.